

```

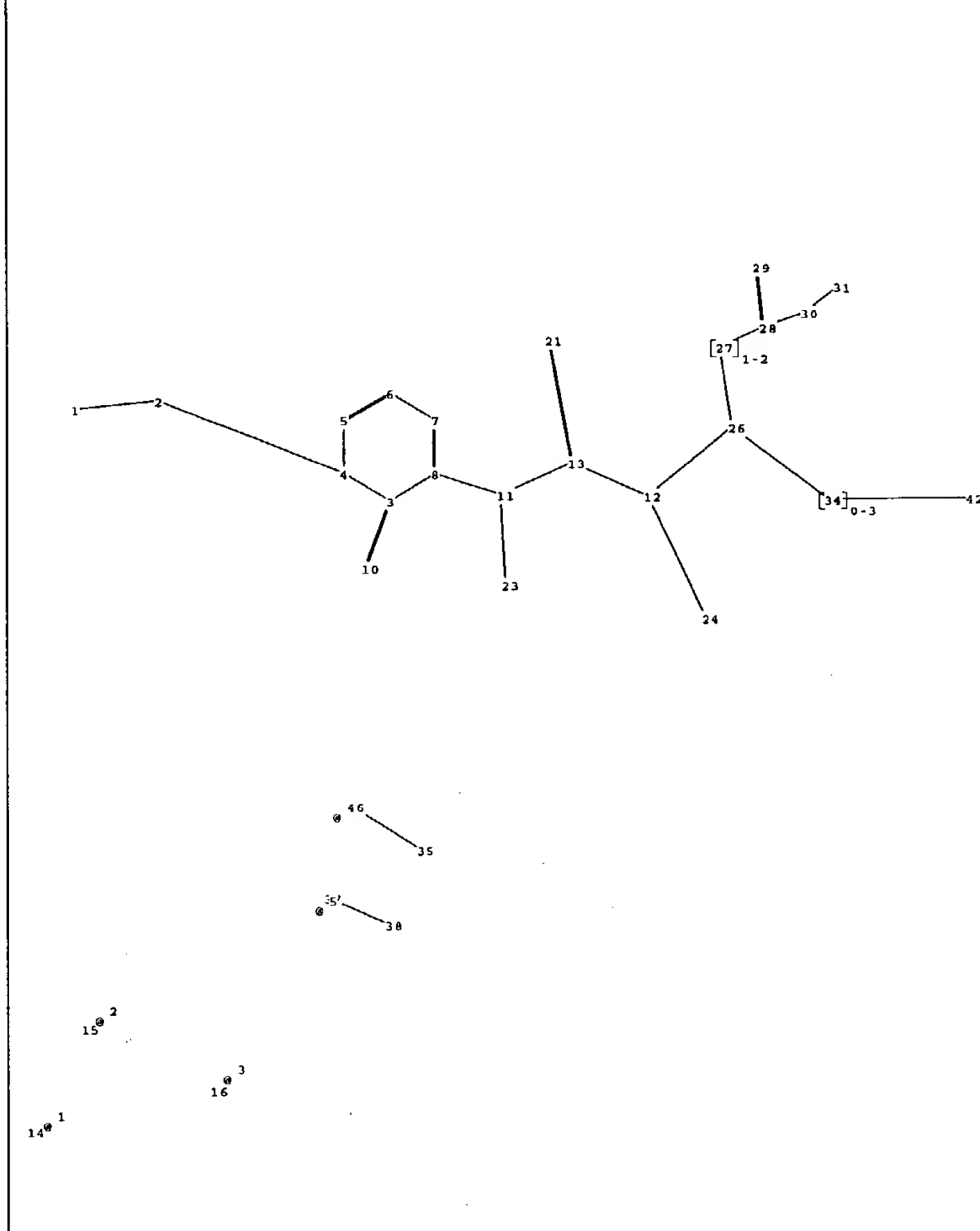
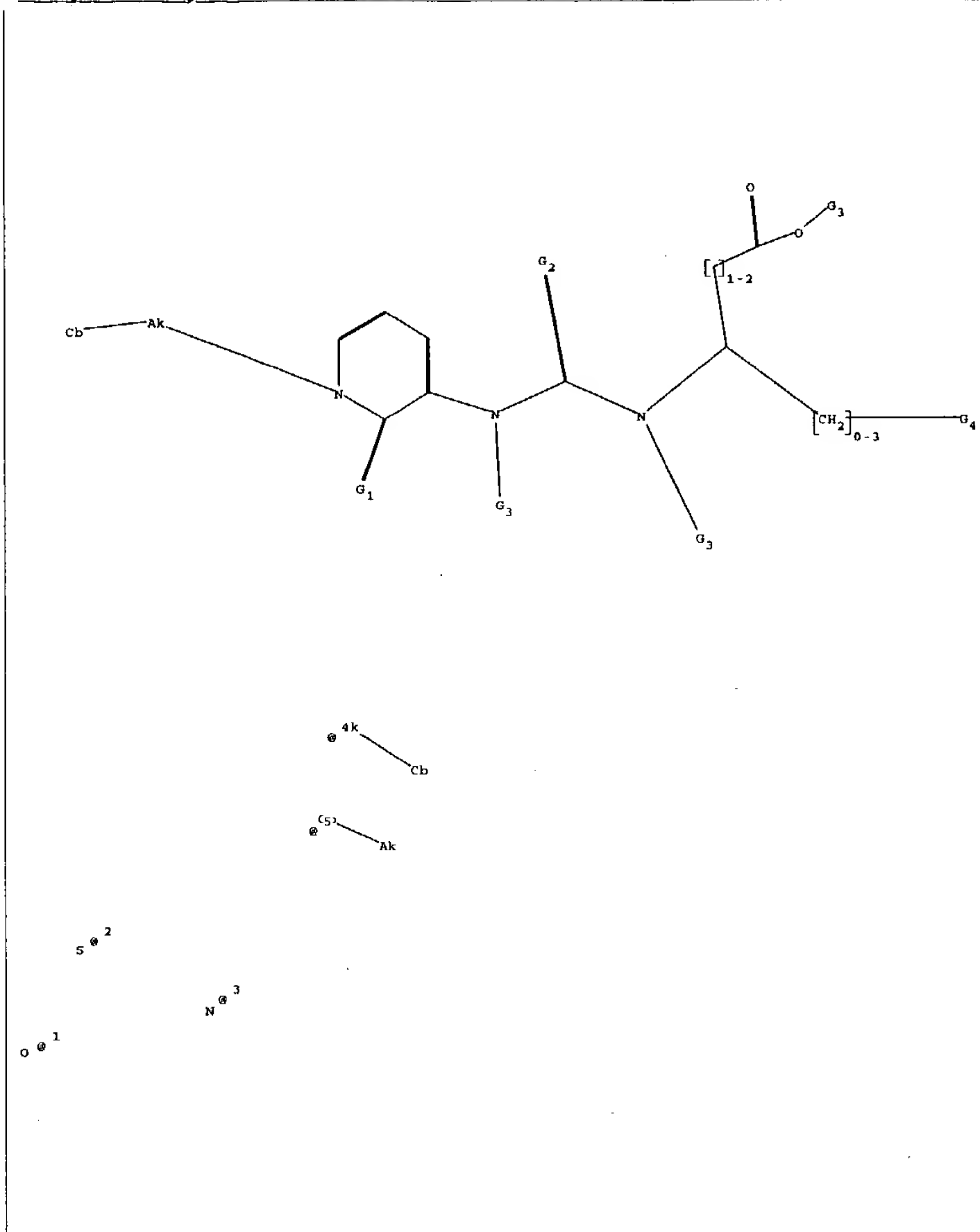
chain nodes :
  1  2 10 11 12 13 14 15 16 21 23 24 26
ring nodes :
  3  4  5  6  7  8
chain bonds :
  1-2  2-4  3-10  8-11 11-13 11-23 12-13 12-24 12-26 13-21
ring bonds :
  3-4  3-8  4-5  5-6  6-7  7-8
exact/norm bonds :
  1-2  2-4  3-4  3-8  3-10  4-5  5-6  6-7  7-8  8-11 11-13 11-23 12-13 12-24 12-26
 13-21

G1:O,S
G2:[*1],[*2],[*3]
G3:H,Ak

Match level :
  1:Atom  2:CLASS  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom 10:CLASS 11:CLASS
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 23:CLASS 24:CLASS 26:CLASS

```

C:\stnweb\Queries\4.str



chain nodes :  
1 2 10 11 12 13 14 15 16 21 23 24 26 27 28 29 30 31 34 35 36 37 38  
42  
ring nodes :  
3 4 5 6 7 8  
chain bonds :  
1-2 2-4 3-10 8-11 11-13 11-23 12-13 12-24 12-26 13-21 26-27 26-34 27-28 28-29  
28-30 30-31 34-42 35-36 37-38  
ring bonds :  
3-4 3-8 4-5 5-6 6-7 7-8  
exact/norm bonds :  
1-2 2-4 3-4 3-8 3-10 4-5 5-6 6-7 7-8 8-11 11-13 11-23 12-13 12-24 12-26  
13-21 28-29 28-30 30-31 34-42 35-36 37-38  
exact bonds :  
26-27 26-34 27-28

G1:O,S

G2:[\*1],[\*2],[\*3]

G3:H,Ak

G4:H,Cb,Ak,[\*4],[\*5]

Match level :

1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 23:CLASS 24:CLASS 26:CLASS  
27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom  
38:CLASS 42:CLASS

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS 4	DEC 08	INPADOC: Legal Status data reloaded
NEWS 5	SEP 29	DISSABS now available on STN
NEWS 6	OCT 10	PCTFULL: Two new display fields added
NEWS 7	OCT 21	BIOSIS file reloaded and enhanced
NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
NEWS 12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS 13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAPLUS
NEWS 14	DEC 17	DGENE: Two new display fields added
NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS 17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAPLUS
NEWS 22	FEB 05	German (DE) application and patent publication number format changes
NEWS 23	MAR 03	MEDLINE and LMEDLINE reloaded
NEWS 24	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS 25	MAR 03	FRANCEPAT now available on STN
NEWS EXPRESS		MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS INTER		General Internet Information
NEWS LOGIN		Welcome Banner and News Items
NEWS PHONE		Direct Dial and Telecommunication Network Access to STN
NEWS WWW		CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:08:44 ON 21 MAR 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 15:08:50 ON 21 MAR 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
 provided by InfoChem.

STRUCTURE FILE UPDATES: 19 MAR 2004 HIGHEST RN 665776-10-3  
 DICTIONARY FILE UPDATES: 19 MAR 2004 HIGHEST RN 665776-10-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> 11

L1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (=>).

=> d 11

L1 HAS NO ANSWERS

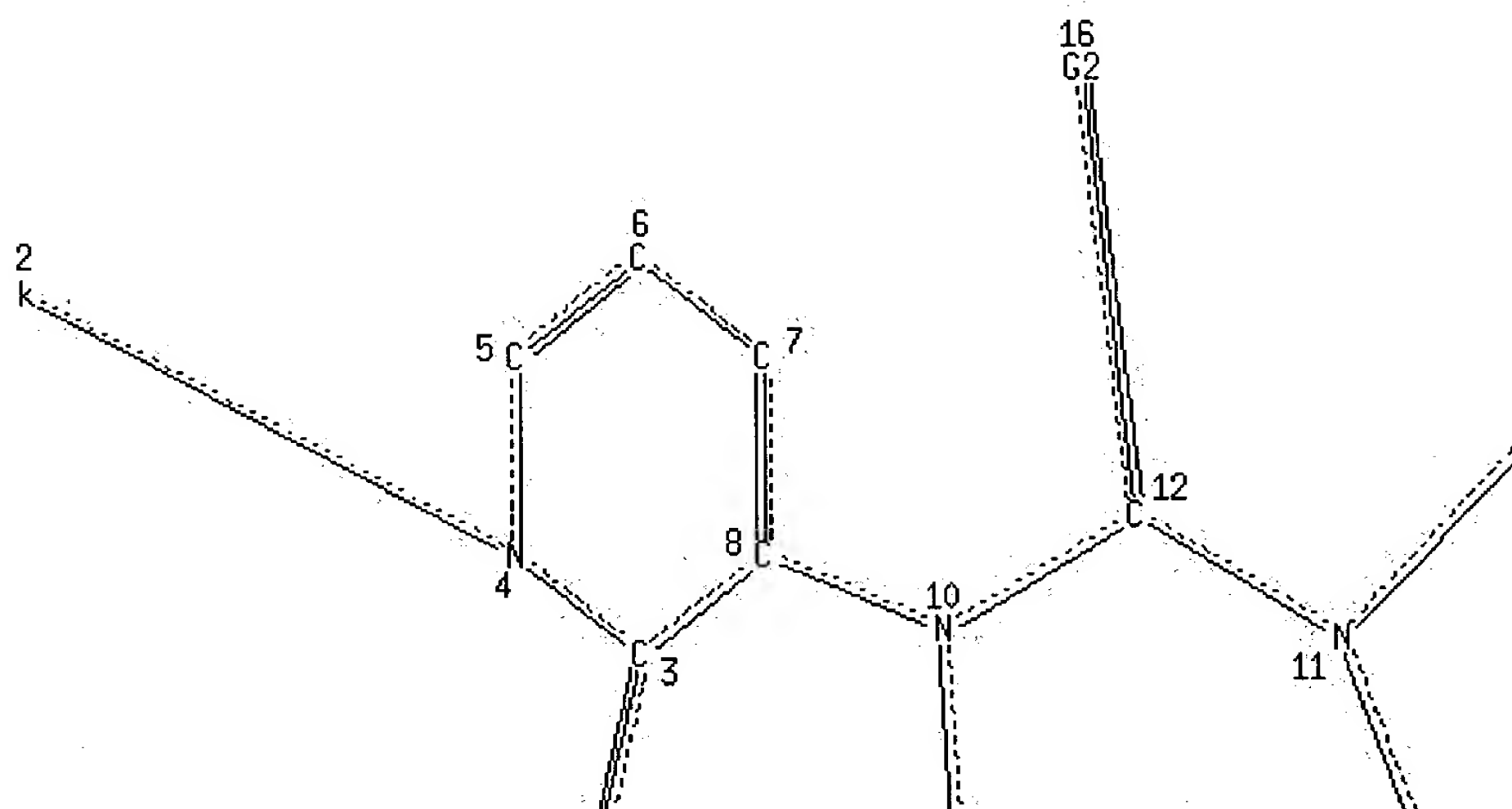
L1 STR

H 22 Ak 23

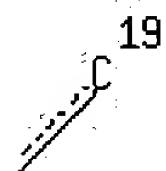
0 20 S 21



Page 1-A



Page 1-B



Page 1-C



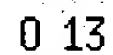
Page 2-B



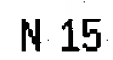
Page 2-C



Page 3-A



Page 4-A



Page 4-B

VAR G1=20/21

VAR G2=13/14/15

VAR G3=22/23

NODE ATTRIBUTES:

NSPEC	IS C	AT	1
NSPEC	IS C	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS C	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12

NSPEC IS C AT 13  
 NSPEC IS C AT 14  
 NSPEC IS C AT 15  
 NSPEC IS C AT 16  
 NSPEC IS C AT 17  
 NSPEC IS C AT 18  
 NSPEC IS C AT 19  
 DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 2 10 11 12 13 14 15 19 20 21 22 23  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

=> s 11  
 SAMPLE SEARCH INITIATED 15:12:21 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 105 TO ITERATE

100.0% PROCESSED 105 ITERATIONS 19 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 1486 TO 2714  
 PROJECTED ANSWERS: 119 TO 641

L2 19 SEA SSS SAM L1

=> s 11 full  
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 15:12:26 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 2405 TO ITERATE

100.0% PROCESSED 2405 ITERATIONS 563 ANSWERS  
 SEARCH TIME: 00.00.01

L3 563 SEA SSS FUL L1

=>  
 L4 STRUCTURE UPLOADED

=> 14  
 L4 IS NOT A RECOGNIZED COMMAND  
 The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (=>).

=> d 14  
 L4 HAS NO ANSWERS  
 L4 STR

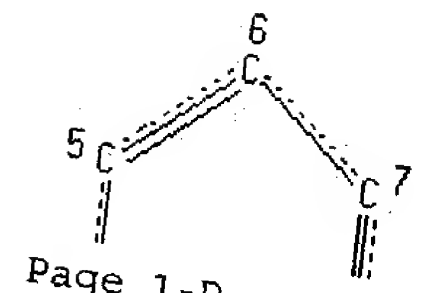
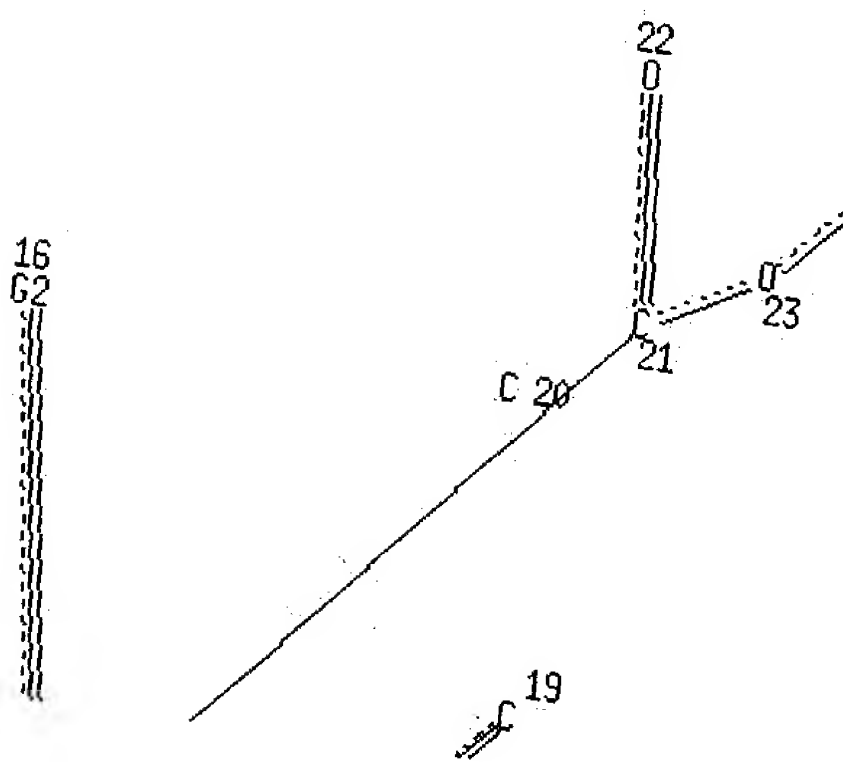
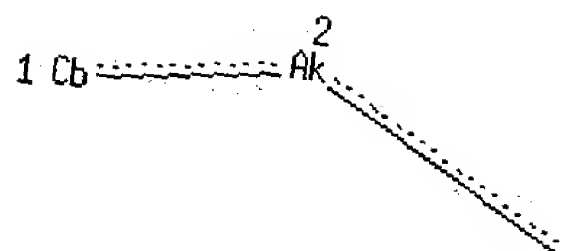
H 37 Cb 38Ak 39

Page 5 of 14

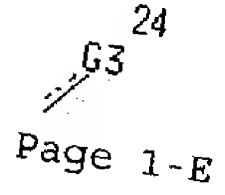
H 35 Ak 36

O 33 S 34

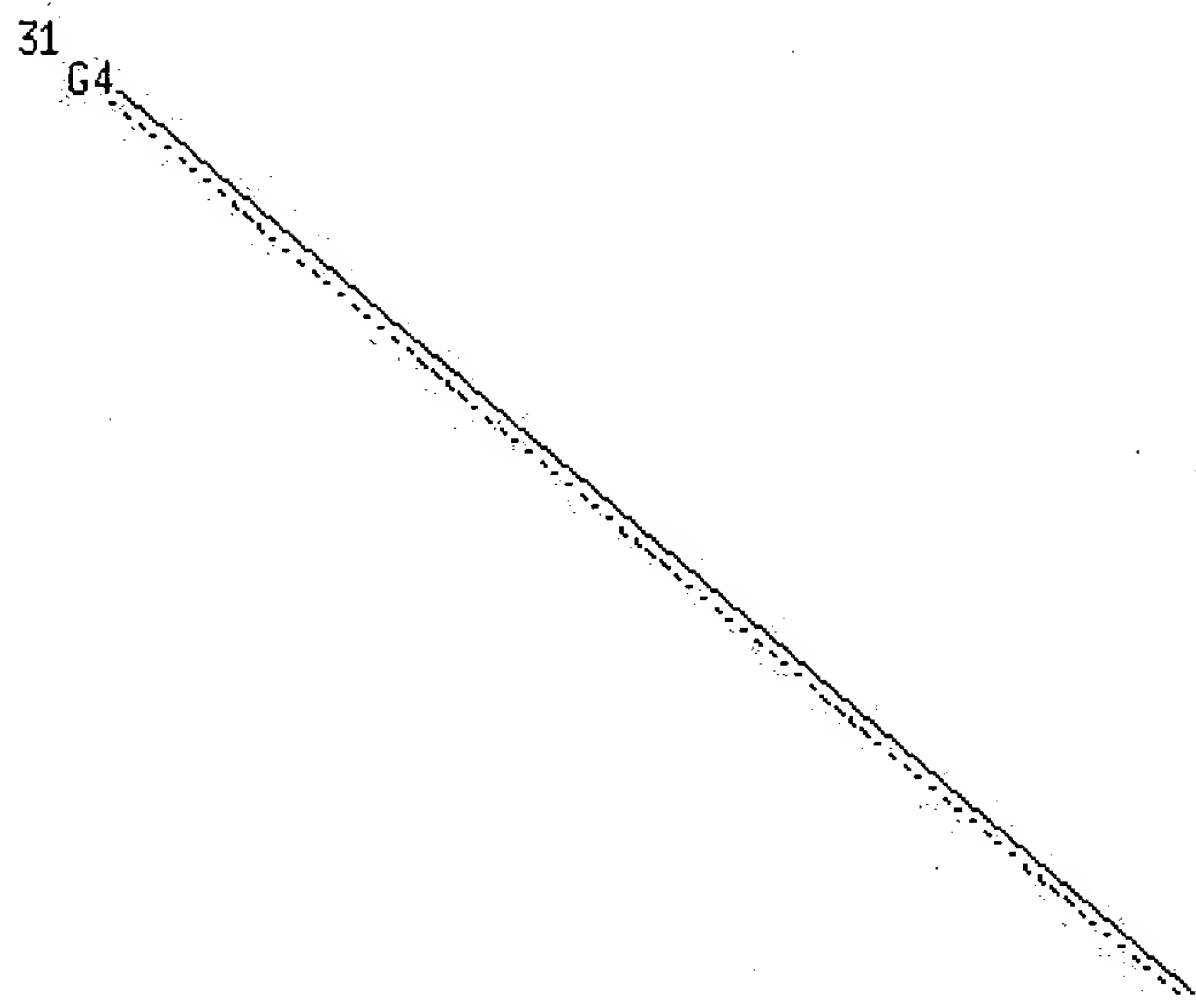
Page 1-C



Page 1-D

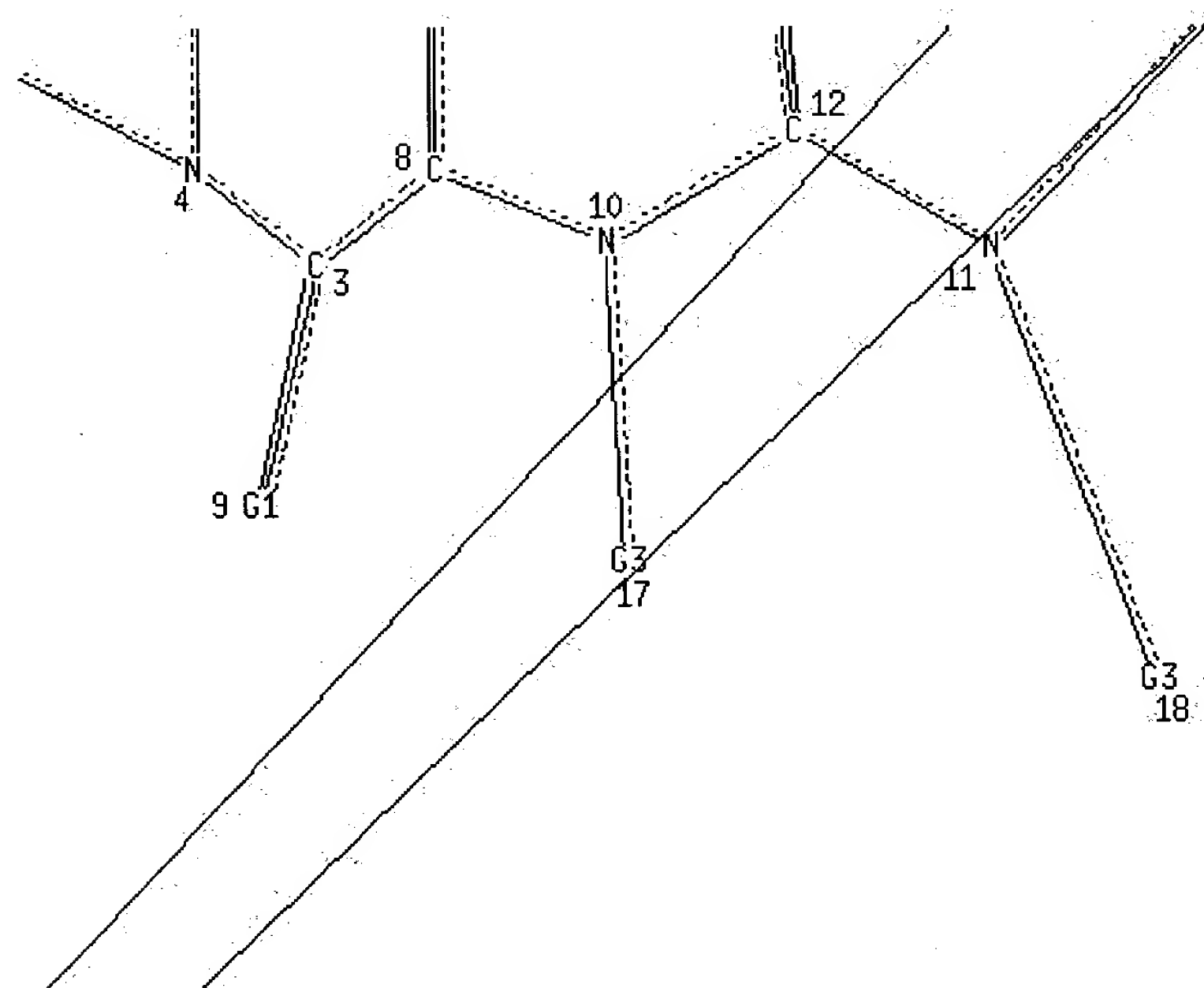


Page 1-E



Page 2-A

Page 2-C



26

Page 2-D

C M2

Page 2-E

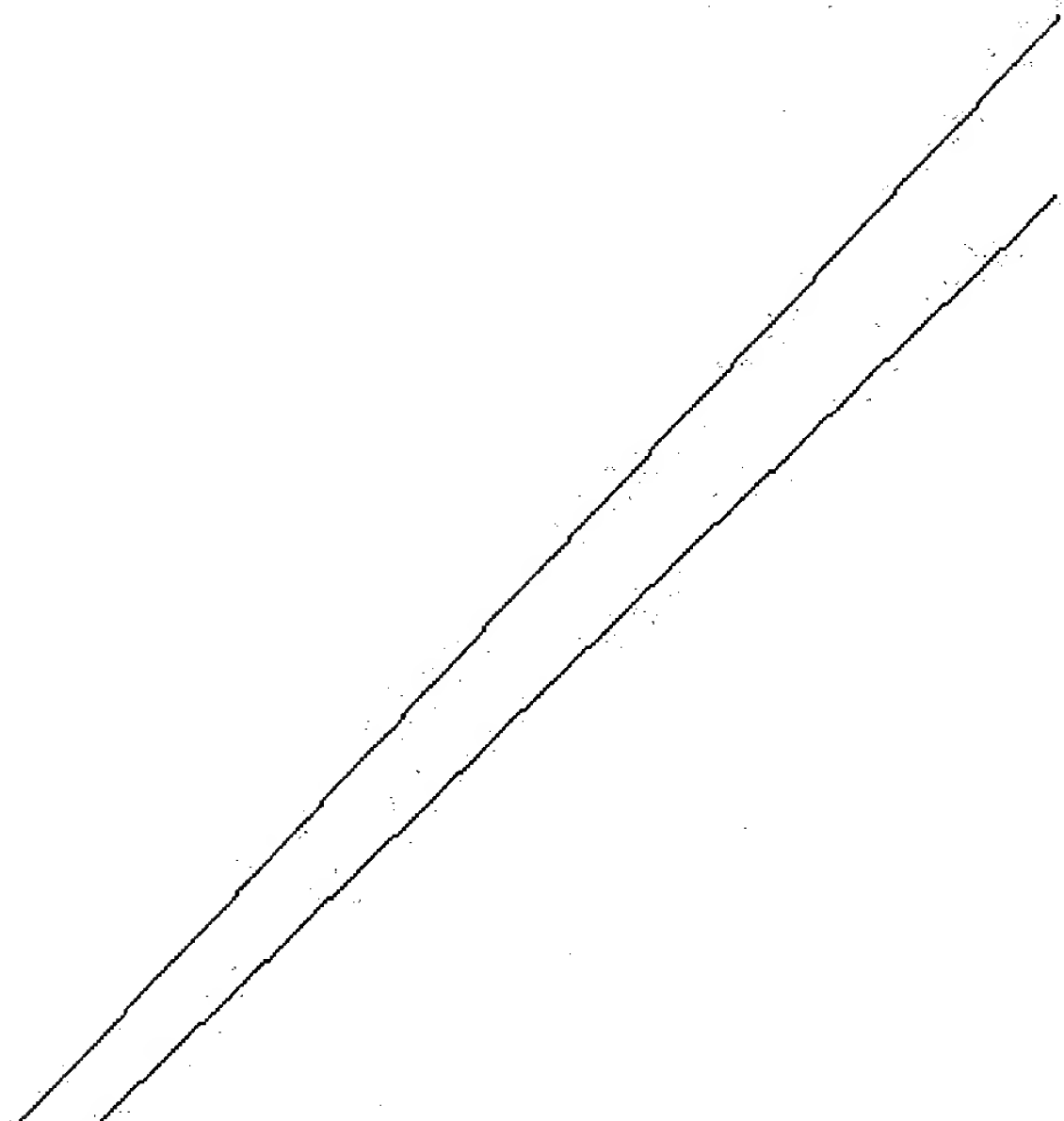




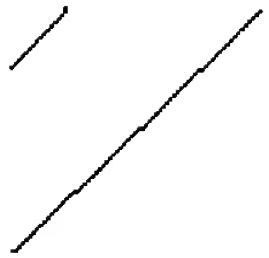
Page 3-A



Page 3-B



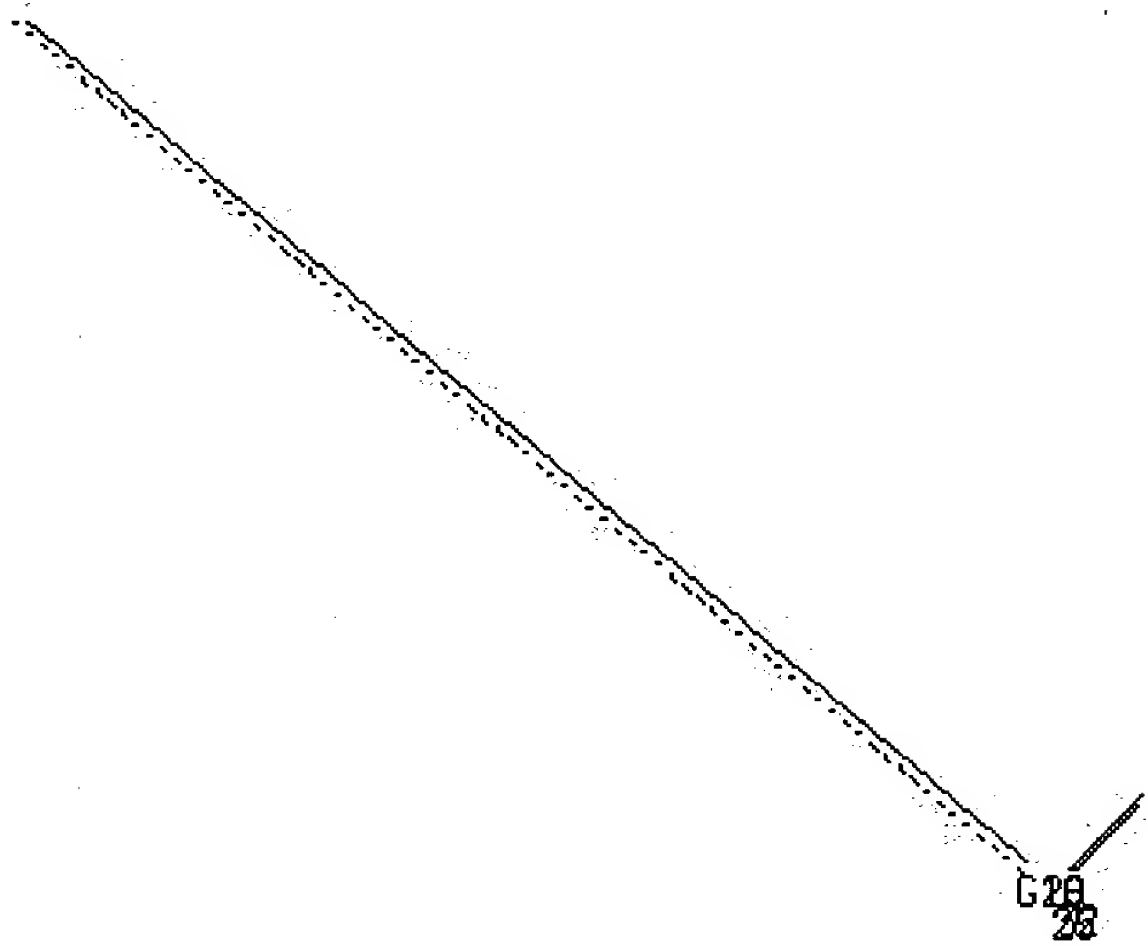
Page 3-C



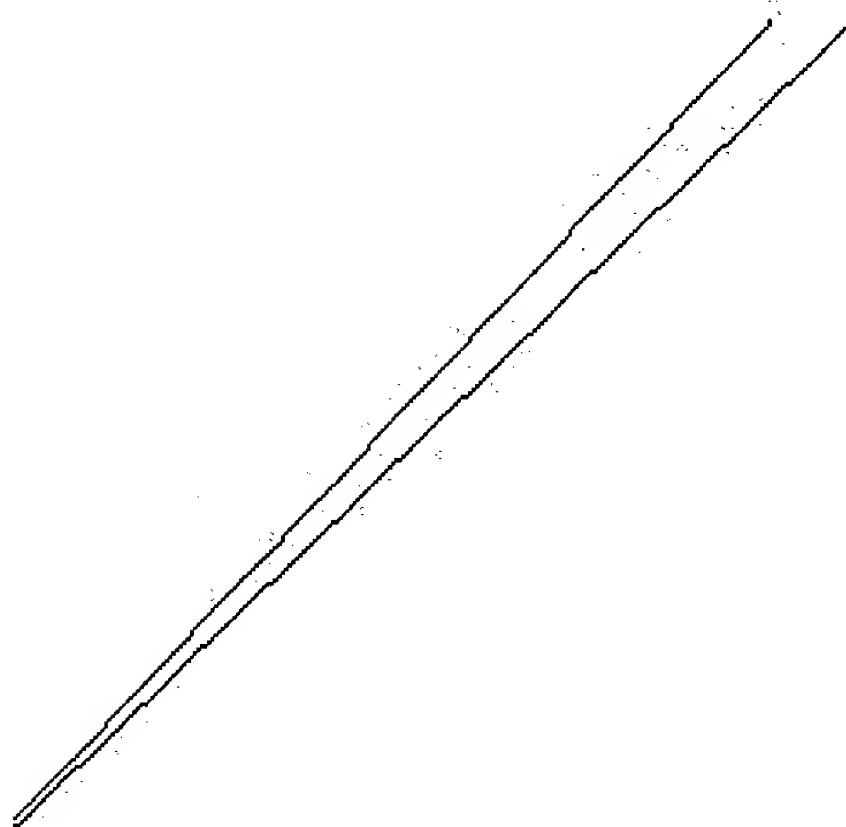
28 Ak  
Cb 27

29 Cb  
Ak 30

Page 3-D



Page 4-B



S 14

N 15

0.13

Page 4-C

VAR G1=33/34

VAR G2=13/14/15

VAR G3=35/36

VAR G4=37/38/39/28/29

REP G19=(0-3) 26-19 26-31

REP G20=(1-2) 20-19 20-21

NODE ATTRIBUTES:

HCOUNT	IS M2	AT	26
NSPEC	IS C	AT	1
NSPEC	IS C	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS C	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17
NSPEC	IS C	AT	18
NSPEC	IS C	AT	19
NSPEC	IS C	AT	20
NSPEC	IS C	AT	21
NSPEC	IS C	AT	22
NSPEC	IS C	AT	23
NSPEC	IS C	AT	24
NSPEC	IS C	AT	25
NSPEC	IS C	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28
NSPEC	IS C	AT	29
NSPEC	IS C	AT	30
NSPEC	IS C	AT	31
NSPEC	IS C	AT	32

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 2 10 11 12 13 14 15 19 20 21 22 23 26 28 30 33 34  
35 36 37 38 39

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

=> s 14

SAMPLE SEARCH INITIATED 15:16:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 42 TO ITERATE

100.0% PROCESSED 42 ITERATIONS

19 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 452 TO 1228

PROJECTED ANSWERS: 119 TO 641

L5 19 SEA SSS SAM L4

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 15:17:03 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1062 TO ITERATE

100.0% PROCESSED 1062 ITERATIONS 554 ANSWERS  
SEARCH TIME: 00.00.01

L6 554 SEA SSS FUL L4

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	315.88	316.09

FILE 'HCAPLUS' ENTERED AT 15:17:07 ON 21 MAR 2004  
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FILE COVERS 1907 - 21 Mar 2004 VOL 140 ISS 13  
FILE LAST UPDATED: 19 Mar 2004 (20040319/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7 2 L6

=> d 17, ibib abs fhitr, 1-2

L7 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
-----------	-------------------

ACCESSION NUMBER:	2002:349146 HCAPLUS
DOCUMENT NUMBER:	136:369608
TITLE:	Preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of $\alpha\beta 1$ integrin binding
INVENTOR(S):	Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde; Decker, Radford E.; Li, Jian
PATENT ASSIGNEE(S):	Texas Biotechnology Corporation, USA
SOURCE:	Eur. Pat. Appl., 131 pp.

CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1203766	A2	20020508	EP 2001-125494	20011106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
ZA 2001008777	A	20030124	ZA 2001-8777	20011024
NO 2001005394	A	20020507	NO 2001-5394	20011105
CN 1412181	A	20030423	CN 2001-145182	20011229
JP 2003119181	A2	20030423	JP 2002-31953	20020208
PRIORITY APPLN. INFO.:			US 2000-707068	A 20001106
			US 2001-973142	A 20011009

OTHER SOURCE(S): MARPAT 136:369608

AB Title compds. were prepd. Thus, 2-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>ZNH<sub>2</sub> (Z = 4-ethyl-2-oxo-1,2-dihydropyridine-1,3-diyl)(prepn. given) was condensed with (S)-4-MeC<sub>6</sub>H<sub>4</sub>CH(NH<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Et and COCl<sub>2</sub> to give, after sapon., (S)-2-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>ZNHCONHCH(C<sub>6</sub>H<sub>4</sub>Me-4)CH<sub>2</sub>CO<sub>2</sub>H (Z as above). Data for biol. activity of title compds. were given.

IT 307520-20-3P

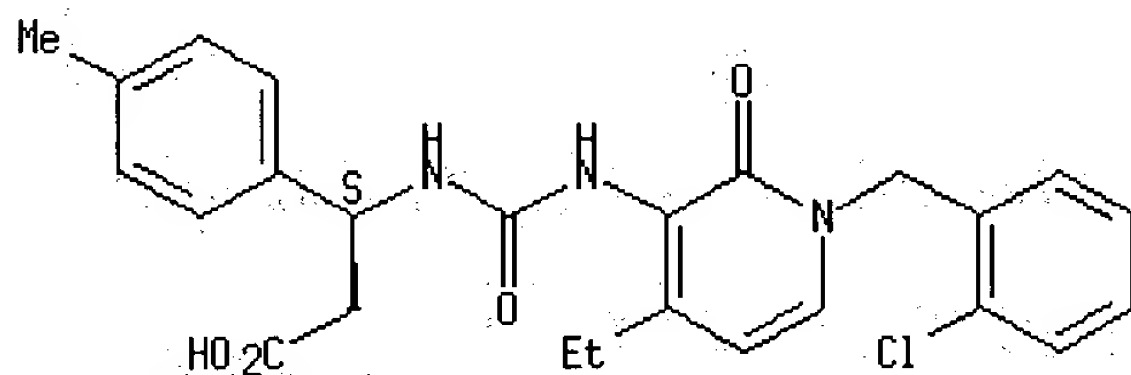
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of  $\alpha 4\beta 1$  integrin binding)

RN 307520-20-3 HCAPLUS

CN Benzenepropanoic acid,  $\beta$ -[[[1-[(2-chlorophenyl)methyl]-4-ethyl-1,2-dihydro-2-oxo-3-pyridinyl]amino]carbonyl]amino]-4-methyl-, ( $\beta$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

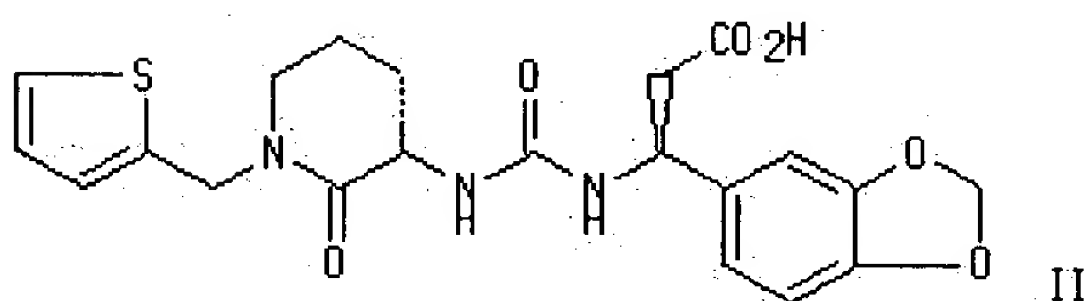
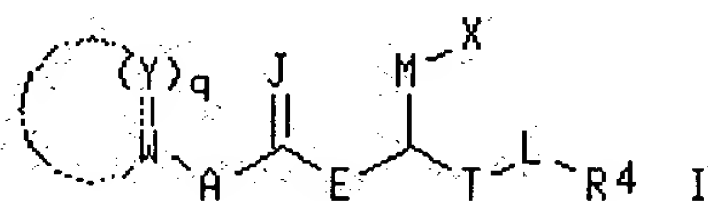
Full Text Citing References

ACCESSION NUMBER: 2000:814302 HCAPLUS  
 DOCUMENT NUMBER: 133:362963  
 TITLE: Preparation of  $\beta$ -amino acid derivatives that inhibit the binding of integrins to their receptors  
 INVENTOR(S): Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde  
 PATENT ASSIGNEE(S): Texas Biotechnology Corporation, USA  
 SOURCE: PCT Int. Appl., 113 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000067746	A1	20001116	WO 2000-US12303	20000505
WO 2000067746	C2	20020829		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1176956	A1	20020206	EP 2000-937527	20000505
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
SI 20744	C	20020630	SI 2000-20021	20000505
BR 2000010293	A	20020716	BR 2000-10293	20000505
JP 2002544161	T2	20021224	JP 2000-616772	20000505
ZA 2001008774	A	20030124	ZA 2001-8774	20011024
NO 2001005418	A	20011221	NO 2001-5418	20011106
PRIORITY APPLN. INFO.:		US 1999-132971P P 19990507		
		WO 2000-US12303 W 20000505		
OTHER SOURCE(S):		MARPAT 133:362963		
GI				



AB Title compds. I [Y, at each occurrence, independently = CO, N, CR<sub>1</sub>, CR<sub>2</sub>R<sub>3</sub>, NR<sub>5</sub>, CH, O, or S; q = 3-10; A = O, S, CR<sub>16</sub>R<sub>17</sub>, NR<sub>6</sub>; E = CH<sub>2</sub>, O, S, NR<sub>7</sub>; J = O, S, NR<sub>8</sub>; M = CR<sub>9</sub>R<sub>10</sub> or (CH<sub>2</sub>)<sub>0-3</sub>; T = CO or (CH<sub>2</sub>)<sub>0-3</sub>; L = O, NR<sub>11</sub>, S, (CH<sub>2</sub>)<sub>0-1</sub>; X = CO<sub>2</sub>B, PO<sub>3</sub>H<sub>2</sub>, SO<sub>3</sub>H, SO<sub>2</sub>NH<sub>2</sub>, SO<sub>2</sub>NHCOR<sub>12</sub>, OPO<sub>3</sub>H<sub>2</sub>, CONHCOR<sub>13</sub>, CONHSO<sub>2</sub>R<sub>14</sub>, tetrazolyl, hydroxyl, H; W = C, CR<sub>15</sub>, N; B, R<sub>1-17</sub> = H, halo, hydroxyl, alkyl, alkoxy, aliph. acyl, CF<sub>3</sub>, nitro, cycloalkyl, alkylheteroaryl, sulfonyl, carboxyl, etc.] or their pharmaceutically acceptable salts were prepd. for inhibition of the binding of  $\alpha 4\beta 1$  integrin to its receptors. Thus, II was prepd. and assayed (IC<sub>50</sub> = 0.2  $\mu$ M) for its ability to suppress binding using a 26-amino acid peptide contg. the CS-1 sequence of fibronectin with N-terminal cysteine coupled to maleimide activated ovalbumin.

IT 307520-20-3P

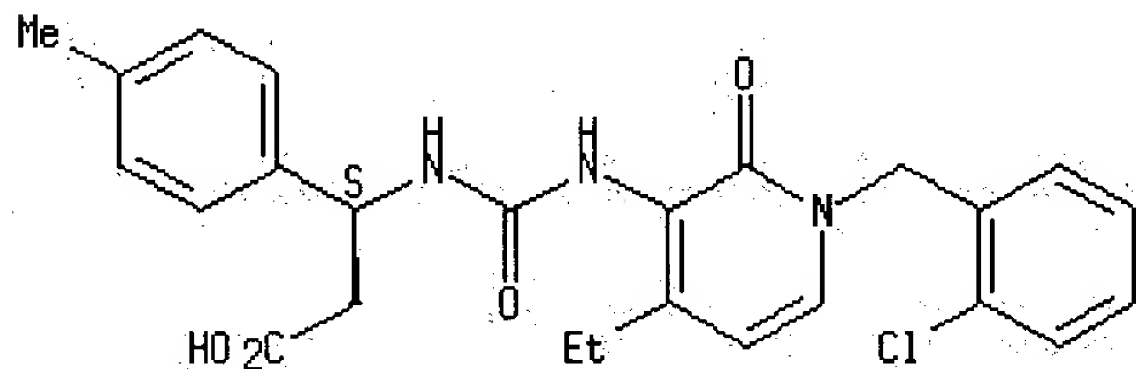
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of  $\beta$ -amino acid derivs. that inhibit the binding of integrins to their receptors)

RN 307520-20-3 HCAPLUS

CN Benzenepropanoic acid,  $\beta$ -[[[1-[(2-chlorophenyl)methyl]-4-ethyl-1,2-dihydro-2-oxo-3-pyridinyl]amino]carbonyl]amino]-4-methyl-, ( $\beta$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

11.87

327.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.39

-1.39

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L1 STRUCTURE UPLOADED

L2 19 S L1

L3 563 S L1 FULL

L4               STRUCTURE UPLOADED  
L5               19 S L4  
L6               554 S L4 FULL

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L7               2 S L6

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L8               0 L6

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